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PASSWORD:

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* * * * * * * * * * Welcome to STN International
                                                   * * * * * * * * * *
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                 Web Page for STN Seminar Schedule - N. America
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                 predefined hit display formats
NEWS 4 APR 28 EMBASE Controlled Term thesaurus enhanced
NEWS 5 APR 28 IMSRESEARCH reloaded with enhancements
NEWS 6 MAY 30 INPAFAMDB now available on STN for patent family
                 searching
NEWS 7 MAY 30 DGENE, PCTGEN, and USGENE enhanced with new homology
                 sequence search option
NEWS 8 JUN 06 EPFULL enhanced with 260,000 English abstracts
NEWS 9 JUN 06 KOREAPAT updated with 41,000 documents
NEWS 10 JUN 13 USPATFULL and USPAT2 updated with 11-character
                 patent numbers for U.S. applications
NEWS 11 JUN 19 CAS REGISTRY includes selected substances from
                 web-based collections
NEWS 12 JUN 25 CA/Caplus and USPAT databases updated with IPC
                 reclassification data
NEWS 13 JUN 30 AEROSPACE enhanced with more than 1 million U.S.
                 patent records
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NEWS 18 JUL 28 EPFULL enhanced with additional legal status
                 information from the epoline Register
NEWS 19 JUL 28 IFICDB, IFIPAT, and IFIUDB reloaded with enhancements
NEWS 20 JUL 28 STN Viewer performance improved
NEWS 21
         AUG 01 INPADOCDB and INPAFAMDB coverage enhanced
NEWS 22 AUG 13 CA/CAplus enhanced with printed Chemical Abstracts
                 page images from 1967-1998
NEWS 23 AUG 15 CAOLD to be discontinued on December 31, 2008
NEWS 24 AUG 15
                 CAplus currency for Korean patents enhanced
NEWS 25 AUG 25 CA/Caplus, CasREACT, and IFI and USPAT databases
                 enhanced for more flexible patent number searching
NEWS 26 AUG 27
                 CAS definition of basic patents expanded to ensure
                 comprehensive access to substance and sequence
                 information
```

NEWS EXPRESS JUNE 27 08 CURRENT WINDOWS VERSION IS V8.3, AND CURRENT DISCOVER FILE IS DATED 23 JUNE 2008.

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ENTRY SESSION 0.84 0.84

TOTAL

SINCE FILE

FULL ESTIMATED COST

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=> D SAV

NAME CREATED NOTES/TITLE

ALL11134628/A 16 AUG 2007 2745 ANSWERS IN FILE CAPLUS

KAREN/A 13 JUL 2007 261 ANSWERS IN FILE CAPLUS SER10534919/A 08 MAY 2008 761 ANSWERS IN FILE CAPLUS STRUCTURE3/A 10 OCT 2007 9741 ANSWERS IN FILE CAPLUS TOTALHITS/A 09 OCT 2007 12338 ANSWERS IN FILE REGISTRY WHOLESET/A 07 JUL 2007 561 ANSWERS IN FILE CAPLUS

=> ACT SER10534919/A

L1 STR

L2 (10295) SEA FILE=REGISTRY SSS FUL L1

L3 761 SEA FILE=CAPLUS L2

=> FIL REG

COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION

FULL ESTIMATED COST 4.80 5.64

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http://www.cas.org/support/stngen/stndoc/properties.html

-> D SAVE
NAME

CREATED

NOTES/TITLE

ALL11134628/A

16 AUG 2007 2745 ANSWERS IN FILE CAPLUS

SER10534919/A

08 MAY 2008 761 ANSWERS IN FILE CAPLUS

STRUCTURE3/A

10 CCT 2007 9741 ANSWERS IN FILE CAPLUS

TOTALHITS/A

09 CCT 2007 12338 ANSWERS IN FILE CAPLUS

TOTALHITS/A

10 DCT 2007 12338 ANSWERS IN FILE CAPLUS

TOTALHITS/A

10 DCT 2007 651 ANSWERS IN FILE CAPLUS

_ .

Uploading C:\Program Files\STNEXP\Queries\10534919\09_02_08_1.str

```
chain nodes:
6 8 10 11
ring nodes:
1 2 3 4 5
chain bonds:
2-8 4-10 5-6 10-11
ring bonds:
1-2 1-5 2-3 3-4 4-5
exact/norm bonds:
1-2 1-5 2-3 2-8 3-4 4-5 4-10 5-6 10-11
```

G1:C,O,S,N

Match level : 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 8:Atom 10:CLASS 11:Atom Generic attributes :

11: Saturation : Unsaturated

L4 STRUCTURE UPLOADED

=> D L4 HAS NO ANSWERS L4 STR

Structure attributes must be viewed using STN Express query preparation.

=> S L4
SAMPLE SEARCH INITIATED 08:35:32 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 33663 TO ITERATE

5.9% PROCESSED 2000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01

23 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 662290 TO 684230
PROJECTED ANSWERS: 6562 TO 8922

L5 23 SEA SSS SAM L4

=> D SCAN

L5 23 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 4-Imidazolidinone, 5-(1H-indol-3-ylmethyl)-3-phenyl-2-thioxoMF C18 B15 N3 O S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> S L4 FUL FULL SEARCH INITIATED 08:35:47 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 679408 TO ITERATE

100.0% PROCESSED 679408 ITERATIONS SEARCH TIME: 00.00.09

6362 ANSWERS

L6 6362 SEA SSS FUL L4

=> FIL CAPLUS

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION

FULL ESTIMATED COST 182.04 187.68

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=> S L6

1296 L6

=> FIL REG

COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION

FULL ESTIMATED COST 1.44 189.12

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=>

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chain nodes:
6 8 10
ring nodes:
1 2 3 4 5 11 12 13 14 15
chain bonds:
2-8 4-10 5-6 10-11
ring bonds:
1-2 1-5 2-3 3-4 4-5 11-12 11-15 12-13 13-14 14-15
exact/norm bonds:
1-2 1-5 2-3 2-8 3-4 4-5 4-10 5-6 10-11 11-12 11-15 12-13 13-14 14-15
```

G1:C,O,S,N

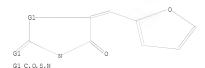
Match level: 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 8:Atom 10:CLASS 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom

L8 STRUCTURE UPLOADED

STR

=> D L8 HAS NO ANSWERS

L8



Structure attributes must be viewed using STN Express query preparation.

=> S L8 FULL SUB=L6

FULL SUBSET SEARCH INITIATED 08:38:19 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED - 208 TO ITERATE

100.0% PROCESSED 208 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

L9 0 SEA SUB=L6 SSS FUL L8

=> S L8 FULL

FULL SEARCH INITIATED 08:38:43 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 36461 TO ITERATE

100.0% PROCESSED 36461 ITERATIONS

13753 ANSWERS

SEARCH TIME: 00.00.01

L10 13753 SEA SSS FUL L8

=> D HIS

(FILE 'HOME' ENTERED AT 08:22:26 ON 02 SEP 2008)

FILE 'CAPLUS' ENTERED AT 08:24:39 ON 02 SEP 2008 ACT SER10534919/A

STR

L2 (10295) SEA FILE=REGISTRY SSS FUL L1

L3 761 SEA FILE=CAPLUS L2

FILE 'REGISTRY' ENTERED AT 08:30:46 ON 02 SEP 2008

L4 STRUCTURE UPLOADED

.5 23 S L4

L6 6362 S L4 FUL

FILE 'CAPLUS' ENTERED AT 08:36:19 ON 02 SEP 2008

L7 1296 S L6

FILE 'REGISTRY' ENTERED AT 08:37:53 ON 02 SEP 2008

L8 STRUCTURE UPLOADED

L9 0 S L8 FULL SUB=L6 L10 13753 S L8 FULL

=>

Uploading C:\Program Files\STNEXP\Queries\10534919\09_02_08_3.str



```
chain nodes:
6 8 10
ring nodes:
1 2 3 4 5 11 12 13 14 15 16 17 18 19 20 21
chain bonds:
2-8 4-10 5-6 10-11 13-16
ring bonds:
1-2 1-5 2-3 3-4 4-5 11-12 11-15 12-13 13-14 14-15 16-17 16-21 17-18
18-19 19-20 20-21
exact/norm bonds:
1-2 1-5 2-3 2-8 3-4 4-5 4-10 5-6 10-11 11-12 11-15 12-13 13-14 13-16
14-15 normalized bonds:
1-6-17 16-21 17-18 18-19 19-20 20-21
```

G1:C,O,S,N

Match level: 1:Atom 2:Atom 4:Atom 5:Atom 6:CLASS 8:Atom 10:CLASS 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom

L11 STRUCTURE UPLOADED

=> D L11 HAS NO ANSWERS L11 STR

Structure attributes must be viewed using STN Express query preparation.

=> S L11 FULL SUB=L10

FULL SUBSET SEARCH INITIATED 08:40:36 FILE 'REGISTRY'

FULL SUBSET SCREEN SEARCH COMPLETED - 9044 TO ITERATE

100.0% PROCESSED 9044 ITERATIONS SEARCH TIME: 00.00.01 8915 ANSWERS

L12 8915 SEA SUB=L10 SSS FUL L11

=> D SCAN

L12 8915 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

IN 4(5H)-Thiazolone, 2-amino-5-[[5-(2-bromo-4-fluorophenyl)-2-

furanyl]methylene]-

MF C14 H8 Br F N2 O2 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L12 8915 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
- IN 2-Furancarboxylic acid, 5-[[5-[[5-(2-methyl-5-nitrophenyl)-2furanyl]methylene]-2,4-dioxo-3-thiazolidinyl]methyl]-, methyl ester
- MF C22 H16 N2 O8 S

PAGE 1-A

PAGE 2-A

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> FIL CAPLUS

COST IN U.S. DOLLARS

COSI IN U.S. DOLLAR

FULL ESTIMATED COST

FULL ESTIMATED COST

266.24

SINCE FILE

ENTRY

TOTAL SESSION 455.36

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Searched by Jason M. Nolan, Ph.D.

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```
=> D HIS
```

L13

115 L12

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FILE 'CAPLUS' ENTERED AT 08:24:39 ON 02 SEP 2008
                ACT SER10534919/A
                STR
L1
L2 (
          10295) SEA FILE=REGISTRY SSS FUL L1
L3
            761 SEA FILE=CAPLUS L2
     FILE 'REGISTRY' ENTERED AT 08:30:46 ON 02 SEP 2008
L4
               STRUCTURE UPLOADED
L5
             23 S L4
L6
           6362 S L4 FUL
     FILE 'CAPLUS' ENTERED AT 08:36:19 ON 02 SEP 2008
           1296 S L6
     FILE 'REGISTRY' ENTERED AT 08:37:53 ON 02 SEP 2008
                STRUCTURE UPLOADED
T.R
L9
              0 S L8 FULL SUB=L6
L10
          13753 S L8 FULL
                STRUCTURE UPLOADED
L11
L12
           8915 S L11 FULL SUB-L10
     FILE 'CAPLUS' ENTERED AT 08:43:11 ON 02 SEP 2008
=> S L12
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(FILE 'HOME' ENTERED AT 08:22:26 ON 02 SEP 2008)

=> S L13 AND COMPOSITION 735831 COMPOSITION

1 L13 AND COMPOSITION

=> D IBIB

L14 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:981372 CAPLUS

DOCUMENT NUMBER: 142:274062

TITLE: Pharmaceutical composition comprising

2-chloro-5-[5-(2-imino-4-oxo-thiazolidin-5-yl

idenemethyl)-furan-2-yl]-benzoic acid derivatives for inhibition of protein tyrosine phosphatase 1b activity

Cho, Jung Myeong; Hwang, Gwang Yeon; Jun, Yeong Ho; INVENTOR(S):

Kim, Jin Hwan; Lee, Tae Gyu; Noh, Seong Gu

PATENT ASSIGNEE(S): Crystalgenomics, Inc., S. Korea SOURCE: Repub. Korean Kongkae Taeho Kongbo, No pp. given

CODEN: KRXXA7 DOCUMENT TYPE: Patent

LANGUAGE: Korean

FAMILY ACC. NUM. COUNT: 1 PATENT INFORMATION:

-----20020614

=> D IBIB ABS HITSTR L14

L14 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:981372 CAPLUS

DOCUMENT NUMBER: 142:274062

TITLE: Pharmaceutical composition comprising

2-chloro-5-[5-(2-imino-4-oxo-thiazolidin-5-yl idenemethyl)-furan-2-yl]-benzoic acid derivatives for

inhibition of protein tyrosine phosphatase 1b activity

INVENTOR(S): Cho, Jung Myeong; Hwang, Gwang Yeon; Jun, Yeong Ho; Kim, Jin Hwan; Lee, Tae Gyu; Noh, Seong Gu

PATENT ASSIGNEE(S): Crystalgenomics, Inc., S. Korea

SOURCE: Repub. Korean Kongkae Taeho Kongbo, No pp. given CODEN: KRXXA7

DOCUMENT TYPE: Patent LANGUAGE: Korean

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

KIND DATE APPLICATION NO. DATE PATENT NO. A 20031224 KR 2002-33284 20020614 KR 2002-33284 20020614 KR 2003095730 PRIORITY APPLN. INFO.:

AB Provided is a pharmaceutical composition comprising 2-chloro-5-[5-(2-imino-4oxo-thiazolidin-5-yl idenemethyl)-furan-2-yl]-benzoic acid derivs. to inhibit the activity of protein tyrosine phosphatase 1B(PTP 1B). It effectively inhibits the activity of PTP 1B and is thus used for the prevention and treatment of obesity or diabetes. A pharmaceutical composition for the inhibit the activity of protein tyrosine phosphatase 1B(PTP 1B) is characterized by comprising 2-chloro-5-[5-(2-imino-4-oxo-thiazolidin-5-yl idenemethyl)-furan-2-yl]-benzoic acid derivs., their pharmaceutically acceptable salt, hydrate, solvate or isomer. In the formula, RI is an aromatic group substituted or unsubstituted with at least one of halogen, alkyloxy, alkyl, amino, alkyl amino, carboxylic acid or amide; a nitrogen, sulfur or oxygen-containing aromatic group; or an aromatic group substituted or unsubstituted C1-C6 alkyl, and R2 is hydrogen; an aromatic group substituted or unsubstituted with at least one of halogen, alkyloxy, alkyl, amino, alkylamino, carboxylic acid or amide; a nitrogen, sulfur or oxygen-containing aromatic group; or an aromatic group substituted or unsubstituted with at least one of halogen, alkyloxy, alkyl, amino, alkylamino, carboxylic acid or amide; a nitrogen, sulfur or oxygen-containing aromatic group; or an aromatic group substituted or unsubstituted C1-C6 alkyl, and R2 is hydrogen.

IT 401611-95-8 401611-95-8D, derivs.

RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses) (pharmaceutical composition comprising furan benzoic acid derivs. for inhibition of protein tyrosine phosphatase 1b activity)

RN 401611-95-8 CAPLUS

CN Benzoic acid, 5-[5-[(2-amino-4-oxo-5(4H)-thiazolylidene)methyl]-2-furanyl]-2-chloro- (CA INDEX NAME)

RN 401611-95-8 CAPLUS

CN Benzoic acid, 5-[5-[(2-amino-4-oxo-5(4H)-thiazolylidene)methyl]-2-furanyl]-2-chloro- (CA INDEX NAME)

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	16.94	472.30
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL
CA SUBSCRIBER PRICE	-0.80	-0.80

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http://www.cas.org/support/stngen/stndoc/properties.html

=> D HTS

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FILE 'CAPLUS' ENTERED AT 08:24:39 ON 02 SEP 2008 ACT SER10534919/A

STR

L1 L2 (10295) SEA FILE=REGISTRY SSS FUL L1

L3 761 SEA FILE=CAPLUS L2

FILE 'REGISTRY' ENTERED AT 08:30:46 ON 02 SEP 2008

STRUCTURE UPLOADED L4

 L_5 23 S L4 1.6 6362 S L4 FUL

FILE 'CAPLUS' ENTERED AT 08:36:19 ON 02 SEP 2008 1296 S L6

FILE 'REGISTRY' ENTERED AT 08:37:53 ON 02 SEP 2008

STRUCTURE UPLOADED T.R

L9 0 S L8 FULL SUB=L6

L10 13753 S L8 FULL L11 STRUCTURE UPLOADED

L12 8915 S L11 FULL SUB-L10

FILE 'CAPLUS' ENTERED AT 08:43:11 ON 02 SEP 2008 L13 115 S L12

L14 1 S L13 AND COMPOSITION

FILE 'REGISTRY' ENTERED AT 08:53:37 ON 02 SEP 2008

=>

Uploading C:\Program Files\STNEXP\Queries\10534919\09_02_08_4.str

```
chain nodes:
6 8 10 22 23 25 26 27
ring nodes:
1 2 3 4 5 11 12 13 14 15 16 17 18 19 20 21
chain bonds:
2-8 4-10 5-6 10-11 13-16 22-23 25-26 25-27
ring bonds:
1-2 1-5 2-3 3-4 4-5 11-12 11-15 12-13 13-14 14-15 16-17 16-21 17-18
18-19 19-20 20-21
exact/norm bonds:
1-2 1-5 2-3 2-8 3-4 4-5 4-10 5-6 10-11 11-12 11-15 12-13 13-14 13-16
14-15 22-23 25-26 25-27
normalized bonds:
16-17 16-21 17-18 18-19 19-20 20-21
```

G1:C,O,S,N

G2:0,S,[*1],[*2]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 8:Atom 10:CLASS 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:CLASS 23:CLASS 25:CLASS 26:CLASS 27:CLASS 26:CLASS 25:CLASS 26:CLASS 25:CLASS 25:CLASS

L15 STRUCTURE UPLOADED

=> D L15 HAS NO ANSWERS

L15



STR



G2 O, S, [@1], [@2]

Structure attributes must be viewed using STN Express query preparation.

=> S L15 FULL SUB=L10

FULL SUBSET SEARCH INITIATED 08:54:30 FILE 'REGISTRY' FULL SUBSET SCREEN SEARCH COMPLETED -9040 TO ITERATE

100.0% PROCESSED 9040 ITERATIONS 6095 ANSWERS

SEARCH TIME: 00.00.01

1.16 6095 SEA SUB=L10 SSS FUL L15

=> D SCAN

L16 6095 ANSWERS

6095 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN 2-Furancarboxylic acid, 5-[(4-[(5-[2-(methoxycarbonyl)phenyl]-2-furanyl]methylene]-2,5-dioxo-1-imidazolidinyl]methyll-, methyl esterIN

C23 H18 N2 O8 MF

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> FIL CAPLUS COST IN U.S. DOLLARS	SINCE FILE ENTRY 43.48	TOTAL SESSION 515.78
FULL ESTIMATED COST		
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-0.80

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FILE COVERS 1907 - 2 Sep 2008 VOL 149 ISS 10 FILE LAST UPDATED: 1 Sep 2008 (20080901/ED)

Caplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2008.

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at: http://www.cas.org/legal/infopolicy.html

=> S L16

L17 107 L16 => D IBIB ABS HISTSR 107 'HISTSR' IS NOT A VALID FORMAT FOR FILE 'CAPLUS' The following are valid formats: ABS ----- GI and AB ALL ----- BIB, AB, IND, RE APPS ----- AI, PRAI BIB ----- AN, plus Bibliographic Data and PI table (default) CAN ----- List of CA abstract numbers without answer numbers CBIB ----- AN, plus Compressed Bibliographic Data CLASS ----- IPC, NCL, ECLA, FTERM DALL ----- ALL, delimited (end of each field identified) DMAX ----- MAX, delimited for post-processing FAM ----- AN, PI and PRAI in table, plus Patent Family data FBIB ----- AN, BIB, plus Patent FAM IND ----- Indexing data IPC ----- International Patent Classifications MAX ----- ALL, plus Patent FAM, RE PATS ----- PI, SO SAM ----- CC, SX, TI, ST, IT SCAN ----- CC, SX, TI, ST, IT (random display, no answer numbers; SCAN must be entered on the same line as the DISPLAY, e.g., D SCAN or DISPLAY SCAN) STD ----- BIB, CLASS

IABS ------ ABS, indented with text labels
IALL ------ ALL, indented with text labels
IBIB ------ BIB, indented with text labels
IMAX ------ MAX, indented with text labels
ISTD ------ STD, indented with text labels
OBIB ------ AN, plus Bibliographic Data (original)
OIBIB ----- OBIB, indented with text labels

SBIB ----- BIB, no citations
SIBIB ----- IBIB, no citations
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HITIND ----- IC, ICA, ICI, NCL, CC and index field (ST and IT) containing hit terms
HITRN ------ HIT RN and its text modification

HITSTR ----- HIT RN, its text modification, its CA index name, and its structure diagram
HITSEQ ----- HIT RN, its text modification, its CA index name, its

structure diagram, plus NTE and SEQ fields
FHITSTR ---- First HIT RN, its text modification, its CA index name, and
its structure diagram

FHITSEQ ---- First HIT RN, its text modification, its CA index name, its

structure diagram, plus NTE and SEQ fields KWIC ----- Hit term plus 20 words on either side

OCC ----- Number of occurrence of hit term and field in which it occurs

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=> D IBIB ABS HITSTR L17 107

L17 ANSWER 107 OF 107 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1972:59507 CAPLUS DOCUMENT NUMBER: 76:59507

ORIGINAL REFERENCE NO.: 76:9589a,9592a

Furan derivatives XXIV. Synthesis of substituted

5-(5-phenyl-2- furfurylidene)rhodanines AUTHOR(S): Krutosikova, A.; Frimm, R.; Kovac, J.

CORPORATE SOURCE: Inst. Org. Chem., Slovak Tech. Univ., Bratislava,

Czech.

Sbornik Prac Chemickej Fakulty SVST (1971), Volume SOURCE .

Date 1969-1970 55-8

CODEN: SCFSAL; ISSN: 0520-7339

DOCUMENT TYPE: Journal

LANGUAGE: Slovak

GI For diagram(s), see printed CA Issue.

AR With the object of preparing biol. active agents of low toxicity, title compds. (I) were prepared by boiling a mixture of the appropriately substituted 5-phenyl-2-furaldehyde, rhodanine, and AcONa in AcOH 30 min. The following I were prepared (R and % yield given): 4-02N, 81; 3-02N, 87; 2-02N, 92; 4-H02C, 87; 4-Cl, 86; 4-Br, 77; 4-Et02C, 80; H, 92; 4-Me, 49;

4-MeO, 51.

ΙT 35274-35-2P 35274-36-3P 35274-37-4P 35274-38-5P 35274-39-6P 35274-40-9P 35274-41-0P 35274-42-1P 35386-81-3P

36405-07-9P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

35274-35-2 CAPLUS RN

4-Thiazolidinone, 5-[[5-(3-nitrophenyl)-2-furanyl]methylenel-2-thioxo-CN (CA INDEX NAME)

- RN 35274-36-3 CAPLUS
- CN 4-Thiazolidinone, 5-[[5-(4-nitrophenyl)-2-furanyl]methylene]-2-thioxo-(CA INDEX NAME)

- RN 35274-37-4 CAPLUS
- CN Benzoic acid, 4-[5-[(4-oxo-2-thioxo-5-thiazolidinylidene)methyl]-2furanyl]- (CA INDEX NAME)

- RN 35274-38-5 CAPLUS
- CN 4-Thiazolidinone, 5-[[5-(4-chlorophenyl)-2-furanyl]methylene]-2-thioxo-(CA INDEX NAME)

- RN 35274-39-6 CAPLUS
- CN 4-Thiazolidinone, 5-[[5-(4-bromophenyl)-2-furanyl]methylene]-2-thioxo-(CA INDEX NAME)

- RN 35274-40-9 CAPLUS
- CN Benzoic acid, 4-[5-[(4-oxo-2-thioxo-5-thiazolidinylidene)methyl]-2furanyl]-, ethyl ester (CA INDEX NAME)

RN 35274-41-0 CAPLUS

CN 4-Thiazolidinone, 5-[(5-phenyl-2-furanyl)methylene]-2-thioxo- (CA INDEX NAME)

RN 35274-42-1 CAPLUS

CN 4-Thiazolidinone, 5-[[5-(4-methylphenyl)-2-furanyl]methylene]-2-thioxo-(CA INDEX NAME)

RN 35386-81-3 CAPLUS

CN 4-Thiazolidinone, 5-[[5-(2-nitrophenyl)-2-furanyl]methylene]-2-thioxo-(CA INDEX NAME)

RN 36405-07-9 CAPLUS

CN 4-Thiazolidinone, 5-[[5-(4-methoxyphenyl)-2-furanyl]methylene]-2-thioxo-(CA INDEX NAME)

=> FIL REG

COST IN U.S. DOLLARS SINCE FILE TOTAL SESSION ENTRY FULL ESTIMATED COST 8.81 524.59 DISCOUNT AMOUNTS (FOR OUALIFYING ACCOUNTS) SINCE FILE TOTAL. SESSION ENTRY CA SUBSCRIBER PRICE -0.80-1.60

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Chain nodes:
6 8 10 11 12 14 15 16 19
ring nodes:
1 2 3 4 5
chain bonds:
2-8 4-10 5-6 10-19 11-12 14-15 14-16
ring bonds:
1-2 1-5 2-3 3-4 4-5
exact/norm bonds:
1-2 1-5 2-3 2-8 3-4 4-5 4-10 5-6 10-19 11-12 14-15 14-16
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G1:C,O,S,N

G2:0,S,[*1],[*2]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 8:Atom 10:CLASS 11:CLASS 12:CLASS 14:CLASS 15:CLASS 16:CLASS 19:Atom Generic attributes:

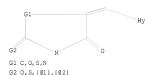
19:

Saturation : Unsaturated

L18 STRUCTURE UPLOADED

=> D L18 HAS NO ANSWERS L18 STR





Structure attributes must be viewed using STN Express query preparation.

=> S L18

SAMPLE SEARCH INITIATED 08:59:36 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED -30616 TO ITERATE

6.5% PROCESSED 2000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01

50 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE** BATCH **COMPLETE** PROJECTED ITERATIONS: 601855 TO 622785 PROJECTED ANSWERS: 47799 TO 53845

L19 50 SEA SSS SAM L18

=> D SCAN

L19 50 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

2,4-Imidazolidinedione, 5-[(2,5-dimethyl-3-furanyl)methylene]-3-[(2-IN

fluorophenyl)methyl]-

C17 H15 F N2 O3 MF

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> S L18 FULL

FULL SEARCH INITIATED 08:59:50 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 617712 TO ITERATE

100.0% PROCESSED 617712 ITERATIONS SEARCH TIME: 00.00.08 50859 ANSWERS

L20 50859 S

50859 SEA SSS FUL L18

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chain nodes:
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ring nodes:
1 2 3 4 5 19 20 21 22 23
chain bonds:
2-8 4-10 5-6 10-19 11-12 14-15 14-16
ring bonds:
1-2 1-5 2-3 3-4 4-5 19-20 19-23 20-21 21-22 22-23
exact/horm bonds:
1-2 1-5 2-3 2-8 3-4 4-5 4-10 5-6 10-19 11-12 14-15 14-16 19-20 19-23
20-21 21-22 22-23
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G1:C,O,S,N

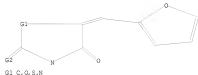
G2:0,S,[*1],[*2]

Match level: 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 8:Atom 10:CLASS 11:CLASS 12:CLASS 14:CLASS 15:CLASS 16:CLASS 19:CLASS 20:Atom 21:Atom 22:Atom 23:Atom

L21 STRUCTURE UPLOADED

=> D L21 HAS NO ANSWERS L21 STR





G2 O, S, [@1], [@2]

Structure attributes must be viewed using STN Express query preparation.

=> S L21 FULL SUB=L20

FULL SUBSET SEARCH INITIATED 09:01:45 FILE 'REGISTRY' FULL SUBSET SCREEN SEARCH COMPLETED -12943 TO ITERATE

100.0% PROCESSED 12943 ITERATIONS

9814 ANSWERS SEARCH TIME: 00.00.01

L22 9814 SEA SUB=L20 SSS FUL L21

=> S L20 NOT L22

L23 41045 L20 NOT L22

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=> S L23 L24 1233 L23

L25

=> S L22

480 L22 => S L25 AND COMPOSITION

735831 COMPOSITION 1.26 8 L25 AND COMPOSITION

=> D IBIB ABS HITSTR L26 TOT

L26 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1994:430177 CAPLUS DOCUMENT NUMBER: 121:30177

ORIGINAL REFERENCE NO.: 121:5497a,5500a

TITLE: Localization of calcium entry through calcium channels

in olfactory receptor neurons using a laser scanning microscope and the calcium indicator dyes Fluo-3 and

Fura-Red

AUTHOR(S): Schild, D.; Jung, A.; Schultens, H. A.

CORPORATE SOURCE: Physiologisches Inst., Univ. Goettingen, Goettingen,

Germany

Cell Calcium (1994), 15(5), 341-8 SOURCE: CODEN: CECADV: ISSN: 0143-4160

DOCUMENT TYPE: Journal LANGUAGE: English

AB The intracellular calcium concentration [Ca2+]i in olfactory receptor neurons of

Xenopus laevis was imaged with high spatial and temporal resolution. A new method using a mixture of the calcium indicator dves Fluo-3 and Fura-Red was employed. The fluorescence patterns in two wavelength bands were measured on the emission side of a confocal laser scanning microscope, and the ratio R of the fluorescence intensities was taken as an estimate of [Ca2+]i. When the neurons were depolarized by elevating the extracellular potassium concentration [K+10 they showed one of three types of responses: a fast

increase

CN

in [Ca2+]i, a slow increase in [Ca2+]i, or no change in [Ca2+]i. The fast increase in [Ca2+]i took place in the soma compartment. For at least 4 s after the onset of depolarization the calcium distribution in the dendrite remained essentially unchanged. To study the fast increase with high time resolution, line scan images were taken. The neurons were depolarized for brief periods applying a solution containing high [K+] onto the soma from an application pipet. The fast increase in [Ca2+]i began with a delay of about 200 ms and went from the resting concentration to about 110 nM above resting concentration Following the depolarization, recovery from elevated [Ca2+]i to resting levels had a time constant of about 15 s. The slow response seemed to depend on the removal of [Na+] from the bath rather than on the elevated [K+] in the bath. The response was also observed with Cd2+, Ni2+, and Co2+ (1.5 mM each) in the bath. The fast increase in [Ca2+li upon depolarization was never seen if R > 0.8 ([Ca2+li > 300 nM). For R < 0.8, 45% of the cells showed a fast response. Cells that responded with a fast increase in [Ca2+]i at low resting [Ca2+]i did not do so for R > 0.8. The authors suggest that the physiol. role of calcium entry through calcium channels on the soma of olfactory cells is to decrease the membrane impedance in an activity dependent way by activating a calcium dependent potassium conductance.

ΤТ 149732-62-7, Fura-Red

RL: ANST (Analytical study)

(Localization of calcium entry through calcium channels in olfactory receptor neurons using a laser scanning microscope and the calcium indicator dyes Fluo-3 and Fura-Red)

RN 149732-62-7 CAPLUS

Glycine, N-[2-[(acetyloxy)methoxy]-2-oxoethyl]-N-[5-[2-[2-[bis[2-bis[2[(acetyloxy)methoxy]-2-oxoethyl]amino]-5-methylphenoxy]ethoxy]-2-[(5-oxo-2thioxo-4-imidazolidinylidene)methyl]-6-benzofuranyl]-, (acetyloxy)methyl ester (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

L26 ANSWER 2 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1994:212943 CAPLUS

DOCUMENT NUMBER: 120:212943

ORIGINAL REFERENCE NO.: 120:37657a,37660a

TITLE: Resting calcium in frog skeletal muscle fibers

estimated with the calcium indicators fluo-3 and fura

red

AUTHOR(S): Harkins, Amy B.

CORPORATE SOURCE: Univ. Pennsylvania, Philadelphia, PA, USA

SOURCE: (1993) 216 pp. Avail.: Univ. Microfilms Int., Order No. DA9321400

From: Diss. Abstr. Int. B 1993, 54(3), 1253

Dissertation

DOCUMENT TYPE: LANGUAGE:

AB Unavailable

IT 149732-62-7, Fura red RL: BIOL (Biological study)

(calcium determination in resting muscle by)

English

RN 149732-62-7 CAPLUS

 ${\tt CN \qquad Glycine, \ N-[2-[(acetyloxy)methoxy]-2-oxoethyl]-N-[5-[2-[2-[bis[2-1]]]]}\\$

[(acetyloxy)methoxy]-2-oxoethyl]amino]-5-methylphenoxy]ethoxy]-2-[(5-oxo-2-thioxo-4-imidazolidinylidene)methyl]-6-benzofuranyl]-, (acetyloxy)methyl ester (CA INDEX NAME)

PAGE 1-A

Searched by Jason M. Nolan, Ph.D.

PAGE 1-B

L26 ANSWER 3 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1993:534716 CAPLUS DOCUMENT NUMBER: 119:134716 ORIGINAL REFERENCE NO.: 119:24077a,24080a

TITLE: Ratiometric confocal calcium measurements with visible wavelength indicators in isolated cardiac myocytes

AUTHOR(S): Lipp, P.; Niggli, E.

CORPORATE SOURCE: Dep. Physiol., Univ. Bern, Bern, Switz. SOURCE: Cell Calcium (1993), 14(5), 359-72

CODEN: CECADV; ISSN: 0143-4160
DOCUMENT TYPE: Journal

LANGUAGE: English

LANGOAGE: English

A new method for ratiometric Ca2+ measurements using indicators with
excitation spectra in the visible range of wavelengths is presented.
Laser-scanning confocal microscopy was used to record intracellular Ca2+
signals with high temporal and spatial resolution in single cardiac myocytes.
The patch-clamp technique was applied to load the cells with the
fluorescent Ca2+ indicators and to follow the membrane currents with the
fluorescence signals simultaneously. Intracellular free Ca2+ concentration
((Ca2+1i) was estimated with a ratiometric method. An in vitro calibration
procedure was used to convert the fluorescence ratio obtained with two
different Ca2+ indicators (Fluo-3 and Fura-Red) into Ca2+ conces. Fluo-3
showed an increase in fluorescence upon a rise in intracellular Ca2+
concentration, while the Fura-Red fluorescence decreased. Since the

fluorescence of Fluo-3 was around 2-fold brighter than the Fura-Red signal the cells were loaded with a 1:2 mixture of the two indicators. The large increase of the fluorescence ratio during a rise in [Ca2+]i (up to 4-fold) allowed time-resolved signals to be recorded with this mixture even when monitored in a very small subcellular volume (around 1 µm3). Long-lasting continuous recordings of the fluorescence were possible because the dye mixture exhibited no detectable bleaching with illumination periods of up to 30 s. The use of the Fluo-3/Fura-Red ratio method should significantly facilitate and improve quant. measurements of [Ca2+]i with high temporal and spatial resolution Moreover, this approach is especially valuable when

used

with confocal microscopes which are usually equipped with lasers in the visible light range. Furthermore, it may be possible to use the same approach with mixts. of other indicators to estimate the concentration of other biol.

- important ions/compds. with a ratiometric calibration.
- T 149732-62-7, Fura Red
 - RL: ANST (Analytical study)

(fluorescence of Fluo-3 and, calcium determination in cardiac myocytes by

ratiometric confocal microscopy in relation to)

149732-62-7 CAPLUS

RN

Glycine, N-[2-[(acetyloxy)methoxy]-2-oxoethyl]-N-[5-[2-[2-[bis[2-[(acetyloxy)methoxy]-2-oxoethyl]amino]-5-methylphenoxy]ethoxy]-2-[(5-oxo-2thioxo-4-imidazolidinylidene)methyl]-6-benzofuranyl]-, (acetyloxy)methyl ester (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

L26 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1993:467007 CAPLUS

DOCUMENT NUMBER: 119:67007

ORIGINAL REFERENCE NO.: 119:11989a,11992a

TITLE: Use of fura red as an intracellular calcium indicator in frog skeletal muscle fibers

Kurebayashi, Nagomi; Harkins, A. B.; Baylor, S. M. AUTHOR(S):

CORPORATE SOURCE: Sch. Med., Univ. Pennsylvania, Philadelphia, PA, 19104-6085, USA

SOURCE: Biophysical Journal (1993), 64(6), 1934-60

CODEN: BIOJAU; ISSN: 0006-3495

DOCUMENT TYPE: Journal LANGUAGE: English

Fura red, a fluorescent Ca2+ indicator with absorbance bands at visible wavelengths, was injected into intact single muscle fibers that had been stretched to a long sarcomere length (.apprx.3.8 μm) and bathed in a 'high-Ca2+' Ringer ([Ca2+] = 11.8 mM). From fura red's slow diffusion

coefficient in myoplasm, 0.16 (± 0.01 , SEM) + 10-6 cm2 s-1 (N = 5;

16°C), it is estimated that apprx.85% of the indicator mols. are bound to muscle constituents of large mol. weight Binding appears to elevate, by 3 to 4-fold, the indicator's apparent dissociation constant for Ca2+ (KD), which is estimated to be 1.1-1.6 μM in myoplasm. Fura red's myoplasmic absorbance spectrum was used to estimate fr, the fraction of fura red mols. in the Ca2+-bound form at rest. In 3 fibers thought to be minimally damaged by the micro-injection, fr was estimated to be 0.15 (10.01). Thus, resting myoplasmic free [Ca2+] ([Ca2+]r) is estimated to be 0.19-0.28 μM. For fibers in normal Ringer solution ([Ca2+] = 1.8 mW), at shorter sarcomere length (.apprx.2.7 μM), and containing a nonperturbing concentration of indicator

(S0.2 mM), [Ca2+]r is estimated to be 0.18-0.27 μM. This range is higher than estimated previously in frog fibers with other techniques. In 6 fibers, R, the indicator's fluorescence ratio signal (equal to the emission intensity measured with 420 mm excitation divided by that measured with 480 mm excitation), was measured at rest and following elec. stimulation and compared with absorbance measurements made from the same fiber region. The anal. implies that RMIN and RMAX (the values of R that would be measured if all indicator mols. were in the Ca2+-free and Ca2+-bound states, resp.) were substantially smaller in myoplasm than in calibration solns. lacking muscle proteins. Several methods for estimation of [Ca2+]r from R are analyzed and discussed.

IT 124903-72-6

HO2C-CH2

RL: ANST (Analytical study)

(in calcium determination in muscle fibers)

RN 124903-72-6 CAPLUS CN Glycine, N-[5-[2-[2-

N Glycine, N-[5-[2-[2-[bis(carboxymethyl)amino]-5-methylphenoxy]ethoxy]-2-[(5-oxo-2-thioxo-4-imidazolidinylidene)methyl]-6-benzofuranyl]-N-(carboxymethyl)- (CA INDEX NAME)

L26 ANSWER 5 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1990:51789 CAPLUS DOCUMENT NUMBER: 112:51789

ORIGINAL REFERENCE NO.: 112:8817a,8820a

TITLE: New tetracarboxylate compounds as fluorescent

intracellular calcium indicators

INVENTOR(S): DeMarinis, Robert M.; Katerinopoulos, Haralambos E.;

Muirhead, Katharine A.

PATENT ASSIGNEE(S): SmithKline Beckman Corp., USA

SOURCE: U.S., 8 pp. CODEN: USXXAM

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1 PATENT INFORMATION:

19
1.5
15
15
19
7
19
15
)

AB Tetracarboxylates I (R = H, AcOCH2; Rl = Me, Et; Z = O, S, NH; Y = NH, S) are chelators for Ca2+ and are useful as fluorescent indicators for measuring intracellular Ca2+ concns. I (R = AcOH2; Rl = Me; Z = O; Y = NH) was prepared from I-(2-amino-4-benzoxylphenoxy)-2-(2-amino-5-methylphenoxy) ethane in 9 steps. AlO smooth muscle cells were loaded with indicator dye and analyzed by fluorescence microscopy. Laser output of 100 mW 488 nm was used to excite the fluorescence of Ca2+-free tetracarboxylate which was collected using a 640-nm longpass filter. Vasopressin-stimulated increase in intracellular Ca2+ caused a decrease in the Ca2+-free form of the carboxylate and therefore a decrease in its 488 nm excited fluorescence.

IT 124903-63-5

RL: ANST (Analytical study)

(fluorescent intracellular calcium indicator)

Τ

- RN 124903-63-5 CAPLUS
- CN Glycine, N-[2-[(acetyloxy)methoxy]-2-oxoethyl]-N-[5-[2-[2-

[[[(acetyloxy)methoxy]methyl][2-[(acetyloxy)methoxy]-2-oxoethyl]amino]-5-methylphenoxy]ethoxy]-2-[(5-oxo2-thioxo-4-inidazolidinylidene)methyl]-6-benzofuranyl]-, (acetyloxy)methyl seter (9CI) (CA INDEX NAME)

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$$\begin{array}{c} & & & & \\ & & & \\ & & & \\ & & & \\ \text{AcO-CH}_2-\text{O-C-CH}_2-\text{N} \\ & & & \\ \end{array}$$

- IT 124903-72-6P
 - RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
- (preparation and reaction of, in preparation of fluorescent intracellular calcium

chelator)

- RN 124903-72-6 CAPLUS
- CN Glycine, N-[5-[2-[2-[bis(carboxymethyl)amino]-5-methylphenoxy]ethoxy]-2-[(5-oxo-2-thioxo-4-imidazolidinylidene)methyl]-6-benzofuranyl]-N-(carboxymethyl)- (CA INDEX NAME)

 HO_2C-CH_2

L26 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1981:609650 CAPLUS DOCUMENT NUMBER: 95:209650

ORIGINAL REFERENCE NO.: 95:34940h,34941a

TITLE: Drug with a cytostatic effect and use of

glycidyl-hydantoin compounds in pharmaceutical

composition

INVENTOR(S): Budnowski, Manfred; Fischer, Herbert

PATENT ASSIGNEE(S): Henkel K.-G.a.A., Fed. Rep. Ger. SOURCE: Ger. Offen., 17 pp.

CODEN: GWXXBX
DOCUMENT TYPE: Patent

DOCUMENT TYPE: Patent LANGUAGE: German

FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

PATENT NO	. KIN	D DATE	APPLICATION NO.		DATE
DE 300335 EP 33503 EP 33503 EP 33503	7 A1 A2 A3 B1	1981081 1982011	2 EP 1981-100544 3		19800131 19810126
AT 22080	T A B2	1986091 1981080		A A A A A A	19810126 19810130 19810131 19800131 19800131 19800310 19800310 19800312 19800312 19800317 19801117

C.

AB Cytostats, I, where R and Rl are the same or different and H or C1-12 hydrocarbon or closed to a ring, and R2 is H or C1-4 alkyl, were prepared and tested in mice inoculated with leukemia P 388 cells. Furfurylidenehydantoin [19628-38-7] and epichlorhydrin [106-89-8] were refluxed with EtMNHPr catalyst for 4-5 h, cooled to 40-50°, mixed with alkali, and H2O was removed by azeotropic distillation After stirring 1 h at 40°, NaCl was removed and epichlorhydrin distilled, and the residue was recrystd. from iso-PrOH to give N,N'-diglycidylfurfurylidenehydantoin [79413-01-7] (yield, 65% of theory).

IT 79413-01-7P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and cytostatic activity of)

RN 79413-01-7 CAPLUS

CN 2,4-Imidazolidinedione, 5-(2-furanylmethylene)-1,3-bis(oxiranylmethyl)-(9CI) (CA INDEX NAME)

IT 19628-38-7

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with epichlorhydrin)

RN 19628-38-7 CAPLUS

CN 2,4-Imidazolidinedione-5-14C, 5-(2-furanylmethylene)- (9CI) (CA INDEX NAME)

L26 ANSWER 7 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1980:41739 CAPLUS DOCUMENT NUMBER: 92:41739

ORIGINAL REFERENCE NO.: 92:6961a,6964a

TITLE: Pharmaceutical composition useful as antidote for heavy metal poisoning

INVENTOR(S): antidote for neavy metal poisoning

Giroux, Eugene L.; Prakash, Nellikunja J.; Schechter,

Paul J.

PATENT ASSIGNEE(S): Merrell Toraude S. A., Fr. SOURCE: Belg., 13 pp.

SOURCE: Belg., 13 pp.
CODEN: BEXXAL
DOCUMENT TYPE: Patent

DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
BE 875232	A1	19790716	BE 1979-194334	19790330
US 4169149	A	19790925	US 1978-892187	19780331
ZA 7901524	A	19800827	ZA 1979-1524	19790330
PRIORITY APPLN. INFO.:			US 1978-892187 A	19780331
			US 1977-765420 A	2 19770121
OTHER SOURCE(S):	MARPAT	92 • 41739		

- AB Mercaptoacrylic acid I (X = CH:CH, O, S, NH; R = H, Me, Et, OH, OMe, OEt, Cl, Br, F, I, CF3) were prepared Thus, 5-trifluoromethylfurfural was treated with rhodamine followed by alkaline hydrolysis to give II (R = CF3). II (R = H) at 25 mg/kg day protected rat against 1 mg/kg day Cd.
- 65712-31-4P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
- (preparation and hydrolysis of) 65712-31-4 CAPLUS RN
- CN
- 4-Thiazolidinone, 2-thioxo-5-[[5-(trifluoromethyl)-2-furanyl]methylene]-(CA INDEX NAME)

L26 ANSWER 8 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1977:38591 CAPLUS

DOCUMENT NUMBER: 86:38591 ORIGINAL REFERENCE NO.: 86:6119a,6122a

TITLE: Nitrofuran-containing composition and its

use as slimicide Hjelte, Nils; Sandberg, Bo INVENTOR(S):

PATENT ASSIGNEE (S): Rexolin Chemicals AB, Swed. SOURCE: Ger. Offen., 18 pp. CODEN: GWXXBX

DOCUMENT TYPE: Patent LANGUAGE: German FAMILY ACC. NUM. COUNT: 1 PATENT INFORMATION:

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	DE 2614798	A1	19761028	DE 1976-2614798	19760406
	FI 7600961	A	19761010	FI 1976-961	19760408
	SE 7604170	A	19761010	SE 1976-4170	19760408
	NO 7601217	A	19761012	NO 1976-1217	19760408
	FR 2307081	A1	19761105	FR 1976-10283	19760408
	FR 2307081	B3	19790105		
PRIO	RITY APPLN. INFO.:			GB 1975-14640 A	19750409

- AB 2-Methylamino-5-(5-nitro-2-furfurylidene)thiazolin-4-one mixture with 3-methyl-2-imino-5-(5-nitro-2-furfurylidene)thiazolidin-4-one [61345-54-8] (I:II = 1:1) is a synergistic bactericide and fungicide suitable for the slime control in paper manufacture Thus 1.2 g I-II mixture/ton paper controlled bacteria and fungi in 2 machines producing 60
- tons of paper daily.
 IT 61345-54-8
 RL: BIOL (Biological study)
- (slimicide for paper manufacture) RN 61345-54-8 CAPLUS
- CN 4(5H)-Thiazolone, 2-(methylamino)-5-[(5-nitro-2-furanyl)methylene]-, mixt. with 2-imino-3-methyl-5-[(5-nitro-2-furanyl)methylene]-4-thiazolidinone (9CI) (CA INDEX NAME)
 - CM 1
 - CRN 25603-06-9 CMF C9 H7 N3 O4 S
- MeNH S CH

CM 2

CRN 25580-69-2 CMF C9 H7 N3 O4 S



=> D IBIB ABS HITSTR L24 1233

L24 ANSWER 1233 OF 1233 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1908:14948 CAPLUS DOCUMENT NUMBER: 2:14948

ORIGINAL REFERENCE NO.: 2:3229h-i,3230a-q

TITLE: Substituted Rhodaninic Acids and their Aldehyde

Condensation Products (VII)

AUTHOR(S): Andreasch, Rudolph

SOURCE: Monatshefte fuer Chemie (1908), 29, 399-419

CODEN: MOCMB7; ISSN: 0026-9247

DOCUMENT TYPE: Journal LANGUAGE: Unavailable

GI For diagram(s), see printed CA Issue.

AB cf. Ibid., 24, 499-27, 1211. m-Tolylthiocarbamic acid, prepared by the interaction of m-toluidine, CS2, and NH3 is, in the form of its NH4 salt, allowed to act upon the Et ester of monochloracetic acid. The resulting v-m-tolylrhodaninic acid (I), m. 148°. In the alcoholic mother

liquor is found the ethyl tolyldithiocarbamylacetate,

MeC5H4.NH.CS.S.CH2.COOC2H5 m. 77°. A number of condensation

products were prepared from this tolvlrhodaninic acid. With BzH was

obtained β-benzylidene-v-m-tolylrhodaninic acid, m. 124°;

with salicylic aldehyde, β-o-oxybenzylidene-v-m-tolylrhodaninic

acid, m. 220°; with m-nitrobenzaldehyde, β-m-nitrobenzylidene-

v-m-tolylrhodaninic acid, m. 234°; with p-dimethyl aminobenzaldehyde, β-dimethyl-p-amidobenzylidene-v-m-

tolvlrhodaninic acid, m. 140°, a compound which dyes wool a

beautiful orange-red; with piperonal, \(\beta\)-methylene-dioxybenzylidene-

v-m-tolylrhodaninic acid, m. 178°; with cinnamic aldehyde,

β-cinnamylidene-v-m-tolylrhodaninic acid, m. 145-6°. When

benzyldithiocarbamic acid, prepared by the action of CS2 upon benzylamine

(2 mol.), is allowed to act upon Et monochloracetate, the final product is

v-benzylrhodaninic acid, m. 83°. As condensation products were prepared: with BzH, β -benzylidene-v-benzylrhodaninic acid, m.

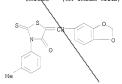
219°; with m-nitrobenzaldehyde, β -m-nitrobenzylidene-vbenzylrhodaninic acid, m. 183°; with p-dimethylaminobenzaldehyde, B-dimethyl-p-aminobenzylidene-v-benzylrhodaninic acid, m. 177°. The action of hydrazine in the presence of CS2 and EtOH gives the hydrazine dithiocarbazinate. The further action of this product upon Et monochloracetate gives v-aminorhodaninic acid (II) m. 92°. From the mother liquor of aminorhodaninic acid was obtained a substance, m. 60°, possibly C10H14O4N2S3. The condensation of aminorhodaninic acid with m-nitrobenzaldehyde gave 8-mnitrobenzylidene-v-aminorhodaninic acid, m. 170°; with p-dimethylaminobenzaldehyde it gave β-dimethyl-p-aminobenzylidenev-aminorhodaninic acid, m. 266°. In analogy with the action of H2CO3 upon the amino acids with the production of the corresponding carbamic acids, the author has substituted CS2 and obtained from these acids the corresponding dithiocarbamic acids. These latter with Et monochloracetate give substituted rhodaninic acids. Thus, from CS2 and glycocoll in Ba(OH)2, to which is finally added a small quantity of EtOH, the compound (III) is formed. The action of Et monochloracetate upon the product gives the vellow Ba rhodaninylacetate (IV). The acid contains 1 H2O, m. 145°. With aldehydes, this acid condenses in the same manner as did the other rhodaninic acids just described. From BzH was obtained β-benzylidenerhodaninylacetic acid, m. 240°; from m-nitrobenzaldehyde, β-m-nitrobenzylidenerhodaninylacetic acid, m. 270-80°; and from p-dimethylaminobenzylaldehyde, β-dimethyl-p-aminobenzylidenerhodaninylacetic acid, m. and decomposes 235°. Other amino acids such as aniline, aminobenzoic acids, etc., give the corresponding rhodaninic acids. In many cases these products are not crystalline.

340966-32-7P, Rhodanine, 5-piperonylidene-3-m-tolyl-

RL: PREP (Preparation) (preparation of)

340966-32-7 CAPLUS RN

CN 4-Thiazolidinone, 5-(1,3-benzodioxol-5-ylmethylene)-3-(3-methylphenyl)-2thioxo- (CA INDEX NAME)



=> D IBIB ABS HITSTR L24 1232

L24 ANSWER 1232 OF 1233 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1910:8921 CAPLUS

DOCUMENT NUMBER: 4:8921

ORIGINAL REFERENCE NO.: 4:1604b-i.1605a-b TITLE: Substituted Rhodaninic Acids and their Aldehyde

Condensation Products. VIII

AUTHOR(S): Kaluza, Ludwig

SOURCE: Graz. Manatsh. (1910), 30, 701-26
DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

Among the substituted acids studied the first under consideration was v-.vphi.-cumylrhodaninic acid (I), prepared by the action of Et monochloroacetate upon NH4 cumyldithiocarbamate. In this reaction a heavy oil separates and gives, upon standing, small colorless crystals, m. 84°, of ethyl .vphi.-cumvldithiocarbamvlacetate, Me3C6H2NHCSSCH2CO2Et, an intermediate product in the rhodaninic acid synthesis. Examinations of the oily substance left after separation of the crystals just mentioned showed that the v-.vphi.-cumylrhodaninic acid was present. It could not, however, be obtained pure. A number of its condensation products with aldehydes were prepared. β-Benzylidene-v-.vphi.-cumylrhodaninic acid, C19H17ONS2, prepared by condensation with BzH, lemon-yellow needles, m. 127°, mol. weight 330.1. β-Methylene-3,4-dioxybenzylidene-v-.vphi.-cumylrhodaninic acid, C20H17O3NS2, by condensation with piperonaldehyde; small needles, m. 188°. β-m-nitrobenzylidene-v-.vphi.-cumylrhodaninic acid, C19H16N2S2O3, from m-nitrobenzaldehyde; vellow crystalline powder, m. 224°. β-p-Nitrobenzylidene-v-.vphi.-cumylrhodaninic acid. C19H16n2S2O3, from p-nitrobenzaldehyde; dark vellow powder, m. 230° (decompose). B-Dimethyl-p-aminobenzylidene-v-.vphi.-cumylrhodaninic acid, C21H22ON2S2, from β-dimethyl-p-aminobenzaldehyde; dark crystalline powder, m. 192°. β -p-Methoxyl-benzylidene-v-.vphi.-cumylrhodaninic acid, C20H1902NS2, from anisic aldehyde; chrome-yellow plates, m. 174°. The second substituted acid was v-isohexylrhodaninic acid (II) prepared from ClCH2CO2Et upon the isohexyl isohexyldithiocarbamate, thick oil, yellow in color. A number of condensation products were prepared: B-benzylidene-visohexylrhodaninic acid, C16H19NS2, from BzH; light yellow needles, m. 87°, mol. weight 282.4. β-m-Nitrobenzylidene-visohexylrhodaninic acid, C16H18O3N2S2, from m-nitrobenzaldehyde; light yellow crystals, m. 166-7°. β-p-Nitrobenzylidene-visohexylrhodaninic acid, C16H18O3N2S2, from p-nitrobenzaldehyde; brown-yellow crystalline powder, m. 130-1°. β-Methylene-3,4dioxybenzylidene-v-isohexylrhodaninic acid, C17H19O3NS2, from piperonaldehyde; gold-yellow flakes, m. 98°. β-Dimethyl-pamino-benzylidene-v-isohexylrhodaninic acid, C18H24ON2S2, from dimethyl-p-aminobenzaldehyde; red needles, m. 140°. B-o-Hydroxybenzylidene-v-isohexylrhodaninic acid, C16H19O2NS2, from salicylic aldehyde, orange-yellow needles, m. 170-2°. β-p-Methoxybenzylidene-v-isohexylrhodaninic acid, C17H21O2NS2, from anisic aldehyde; chrome-yellow needles, m. 85°. B-Cinnamylene-v-isohexylrhodaninic acid, C18H21ONS2, from cinnamic aldehyde, vellow scales, m. 129-31°. The action of Et chlorocarbonate from the isohexvlisohexvldithiocarbamate was found to give isohexylisothiocyanate, C17H13NS, yellow oil, b. p. 208-9°. By the action of NH3 and EtOH it gives a white crystalline isohexylthiourea, C7H16N2S, m. 62°. With isohexylamine instead of NH3 diisohexylthiourea, C13H28N2S, crystallizing in glancing white leaflets, m. 46°, was obtained. The action of (CN)2 on isohexylthiourea and the subsequent treatment of this cyanide with HCl gave a monoisohexylthioparabanic acid (III), C9H14N2O2S; light yellow crystals m. 110°, mol. weight 197. When this product is treated with AgNO3 in EtOH or H2O, with final mixing, there was extracted by Et2O a monoisohexylparabanic acid, C9H14N2O3; small white crystals, m. 76°. In a similar manner the diisohexylthiourea was made to give

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diisohexylthioparabanic acid, C15H26O2N2S; lemon-yellow needles, m.
     40°. This in turn gave diisohexylparabanic acid, which however
     could not be prepared pure or in crystalline form.
     859960-24-0P, Rhodanine, 5-piperonylidene-3-pseudocumyl-
     860757-30-8P, Rhodanine, 3-isohexyl-5-piperonylidene-
     RL: PREP (Preparation)
        (preparation of)
RN
     859960-24-0 CAPLUS
CN
     4-Thiazolidinone, 5-(1,3-benzodioxol-5-ylmethylene)-2-thioxo-3-(2,3,5-
     trimethylphenyl) - (CA INDEX NAME)
  S
Me
Me
           Me
                 CAPLUS
     860757-30-8
     4-Thiazolidinane, 5-(1,3-benzodioxol-5-ylmethylene)-3-(4-methylpentyl)-2-
            (CA INDEX NAME)
     thioxo-
MeoCH- (CHo) 3
=> D IBIB ABS HITSTR L24 1231
L24 ANSWER 1231 OF 1233 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:
                         1911:9676 CAPLUS
DOCUMENT NUMBER:
                         5:9676
ORIGINAL REFERENCE NO.:
                        5:1756b-i,1757a
TITLE:
                         Substituted Rhodanines and their Aldehyde Condensation
                         Products. X
AUTHOR(S):
                         Andreasch, Rudolf
SOURCE:
                         Monatshefte fuer Chemie (1911), 31, 785-95
                         CODEN: MOCMB7: ISSN: 0026-9247
DOCUMENT TYPE:
                         Journal
LANGUAGE:
                         Unavailable
    For diagram(s), see printed CA Issue.
    cf. C. A., 2, 3229. Dithiocarbaminoacetic acid HS2CNHCH2CO2H, is best
     prepared from aminoacetic acid, CS2 and NH3, in dilute alc., the product
     consists of diammonium dithiocarbaminoacetate; white needles with 1H2O, m.
     110° (gas evolution). Yield, about 80%. In a similar manner,
     alanine forms diammonium α-dithiocarbaminopropionate,
    NH4S2CNHCHMeCO2NH4; long needles with 1H2O, m. 128-9° (decompose and
     gas evolution). When treated with HCl, or H2SO4 and Et2O it gives
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a-rhodaninepropionic acid formula (I) below; warty crystals from alc., m. 127°. The above condensation may also be realized by the use of KOH, or Ba(OH)2 in place of NH3. β -Benzylidene- α rhodaninepropionic acid (II), from (I) and BzH, in Et20; light yellow needles, or warty aggregates from alc., m. 191°. β-p-Dimethylaminobenzylidene-α-rhodaninepropionic acid (III), from (I) and p-dimethyl-aminobenzaldehyde; needles, or crusts resembling CrO3 in color, m. 210-20°. It dyes the skin, wool and silk orange-red, but the colors are not very fast towards light. β-p-Hydroxybenzylidene-α-rhodaninepropionic acid (IV), from (I) and p-hydroxybenzaldehyde; light chrome-yellow needles or crusts, softens 190°, m. 205-10°. β-Methylenedioxybenzylidene-αrhodaninepropionic acid, (V), from (I) and piperonaldehyde in AcOH; orange-yellow warts from alc. or Et20, m. 197-9°. When glycylglycine hydrochloride is treated with CS2 and aqueous NH3 it appears to form the di-NH4 dithiocarbamate, NH4S2CNHCH2CONHCH2CO2NH4. It was not purified but was heated with chloroacetic ester and the product acidified and extracted with Et20. The resulting compound consists of rhodanineglycylglycine (IV); yellow syrup. With BzH, in AcOH, it forms B-benzylidenerhodanineglycylgycine (VII); greenish vellow scales, or needles, softens 180°, m. 190°. The rhodanines from asparagine, aspartic and glutamic acids and synthetic leucine, both optically active and inactive, are all oils, as are likewise their condensation products with aldehydes. As these oils decompose when heated the compds. in question could not be purified.

IT 300812-43-5P, 3-Thiazolidineacetic acid, 4-keto-α-methyl-5-piperonylidene-2-thio-

RL: PREP (Preparation) (preparation of)

RN 300812-43-5 CAPLUS

CN 3-Thiazolidineacetic acid, 5-(1,3-benzodioxol-5-ylmethylene)-amethyl-4-oxo-2-thioxo- (CA INDEX NAME)

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Uploading C:\Program Files\STNEXP\Queries\10534919\09_02_08_7.str





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chain nodes: 6 8 10 11 12 14 15 16
ring nodes: 1 2 3 4 5 19 20 21 22 23 24 25 26 27
chain bonds: 2-8 4-10 5-6 10-19 11-12 14-15 14-16
ring bonds: 1-2 1-5 2-3 3-4 4-5 19-20 19-24 20-21 21-22 21-25 22-23 22-27 23-24
25-26 26-27
exact/norm bonds: 1-2 1-5 2-3 2-8 3-4 4-5 4-10 5-6 10-19 11-12 14-15 14-16 21-25 22-27
rormalized bonds: 1-2 19-24 20-21 21-22 22-23 23-24
```

G1:C,O,S,N

G2:0,S,[*1],[*2]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 8:Atom 10:CLASS 11:CLASS 12:CLASS 14:CLASS 15:CLASS 15:CLAS

L27 STRUCTURE UPLOADED

=> D L27 HAS NO ANSWERS L27 STR





G1 C, O, S, N

G2 O, S, [@1], [@2]

Structure attributes must be viewed using STN Express query preparation.

=> S L27 FULL SUB=L23

REG1stRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress... Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

FULL SUBSET SEARCH INITIATED 09:10:12 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED - 2970 TO ITERATE

100.0% PROCESSED 2970 ITERATIONS

2111 ANSWERS

SEARCH TIME: 00.00.01

L28 2111 SEA SUB=L23 SSS FUL L27

SUBSET IS IGNORED AS A SCOPE FOR THIS SEARCH

164 L28

=> D IBIB ABS HITSTR L29 164

L29 ANSWER 164 OF 164 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1908:14948 CAPLUS DOCUMENT NUMBER: 2:14948

ORIGINAL REFERENCE NO.: 2:3229h-i,3230a-g

TITLE:

Substituted Rhodaninic Acids and their Aldehyde Condensation Products (VII)

AUTHOR(S): Andreasch, Rudolph

SOURCE: Monatshefte fuer Chemie (1908), 29, 399-419

CODEN: MOCMB7; ISSN: 0026-9247

DOCUMENT TYPE: Journal Unavailable

LANGUAGE:

For diagram(s), see printed CA Issue.

cf. Ibid., 24, 499-27, 1211. m-Tolylthiocarbamic acid, prepared by the interaction of m-toluidine, CS2, and NH3 is, in the form of its NH4 salt, allowed to act upon the Et ester of monochloracetic acid. The resulting v-m-tolylrhodaninic acid (I), m. 148°. In the alcoholic mother liquor is found the ethyl tolyldithiocarbamylacetate, MeC5H4.NH.CS.S.CH2.COOC2H5 m. 77°. A number of condensation products were prepared from this tolylrhodaninic acid. With BzH was obtained β-benzylidene-v-m-tolylrhodaninic acid, m. 124°; with salicylic aldehyde, β-o-oxybenzylidene-v-m-tolylrhodaninic acid, m. 220°; with m-nitrobenzaldehyde, β-m-nitrobenzylidenev-m-tolylrhodaninic acid, m. 234°; with p-dimethyl aminobenzaldehyde, B-dimethyl-p-amidobenzylidene-v-mtolylrhodaninic acid, m. 140°, a compound which dyes wool a beautiful orange-red; with piperonal, \(\beta\)-methylene-dioxybenzylidenev-m-tolylrhodaninic acid, m. 178°; with cinnamic aldehyde, B-cinnamylidene-v-m-tolylrhodaninic acid, m. 145-6°. When benzyldithiocarbamic acid, prepared by the action of CS2 upon benzylamine (2 mol.), is allowed to act upon Et monochloracetate, the final product is v-benzylrhodaninic acid, m. 83°. As condensation products were prepared: with BzH, β-benzylidene-v-benzylrhodaninic acid, m. 219°; with m-nitrobenzaldehyde, β-m-nitrobenzylidene-vbenzylrhodaninic acid, m. 183°; with p-dimethylaminobenzaldehyde, B-dimethyl-p-aminobenzylidene-v-benzylrhodaninic acid, m. 177°. The action of hydrazine in the presence of CS2 and EtOH gives the hydrazine dithiocarbazinate. The further action of this product upon Et monochloracetate gives v-aminorhodaninic acid (II) m. 92°. From the mother liquor of aminorhodaninic acid was obtained a substance, m. 60°, possibly C10H14O4N2S3. The condensation of aminorhodaninic acid with m-nitrobenzaldehyde gave 8-mnitrobenzylidene-v-aminorhodaninic acid, m. 170°; with p-dimethylaminobenzaldehyde it gave β -dimethyl-p-aminobenzylidene-v-aminorhodaninic acid, m. 266°. In analogy with the action of H2CO3 upon the amino acids with the production of the corresponding

carbamic acids, the author has substituted CS2 and obtained from these

```
acids the corresponding dithiocarbamic acids. These latter with Et
    monochloracetate give substituted rhodaninic acids. Thus, from CS2 and
     glycocoll in Ba(OH)2, to which is finally added a small quantity of EtOH,
     the compound (III) is formed. The action of Et monochloracetate upon the
     product gives the yellow Ba rhodaninylacetate (IV). The acid contains 1
     H2O, m. 145°. With aldehydes, this acid condenses in the same
    manner as did the other rhodaninic acids just described. From BzH was
     obtained β-benzylidenerhodaninylacetic acid, m. 240°; from
    m-nitrobenzaldehyde, β-m-nitrobenzylidenerhodaninylacetic acid, m.
     270-80°; and from p-dimethylaminobenzylaldehyde,
    β-dimethyl-p-aminobenzylidenerhodaninylacetic acid, m. and decomposes
     235°. Other amino acids such as aniline, aminobenzoic acids, etc.,
     give the corresponding rhodaninic acids. In many cases these products are
     not crystalline.
     340966-32-7P, Rhodanine, 5-piperonylidene-3-m-tolyl-
     RL: PREP (Preparation)
       (preparation of)
     340966-32-7 CAPLUS
     4-Thiazolidinone, 5-(1,3-benzodioxol-5-vlmethylene)-3-(3-methylphenyl)-2-
     thioxo- (CA INDEX NAME)
=> S L24 NOT L29
L30
         1069 L24 NOT L29
=> D IBIB ABS HITSTR L30 1069
L30 ANSWER 1069 OF 1069 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:
                        1924:16150 CAPLUS
DOCUMENT NUMBER:
                         18:16150
ORIGINAL REFERENCE NO.: 18:2166d-e
TITLE:
                        Use of rhodanine in organic syntheses. IV. Indole- and
                         furvlpvroracemic acids
                         Granacher, Ch.; Gero, M.; Schelling, V.
AUTHOR(S):
                         Helvetica Chimica Acta (1924), 7, 575-8
SOURCE:
                         CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE:
                         Journal
LANGUAGE:
                         Unavailable
    cf. C. A. 17, 2424. β-Indolalrhodanine, glistening brown leaflets,
     which gradually decompose above 200°. Heated with 10% KOH for 1-2
     hrs., it gives β-indole-α-sulfhydryl-acrylic acid,
     orange-yellow, decomps. 190°. The NH4OH solution gives with FeCl3 a
     typical dark green color. With concentrated NH4OH on the H2O bath this gives
     β-indole-pyroracemic acid (Ellinger and Matsuoka, C. A. 16, 951).
     Furylsulfhydrylacrylic acid cannot be directly changed into
```

RN

Me

furylpyroracemic acid, m. 131° , by heating with NH3 but is transformed into the oxime and this is decomposed by H2SO8. The acid is very unstable and in a few days gives a greenish yellow or dark resinous mass.

TT 73855-59-1P, Rhodanine, 5-(3-indylmethylene)-

RL: PREP (Preparation)
(preparation of)

RN 73855-59-1 CAPLUS

CN 4-Thiazolidinone, 5-(1H-indol-3-ylmethylene)-2-thioxo- (CA INDEX NAME)

=> D IBIB ABS HITSTR L30 1068

L30 ANSWER 1068 OF 1069 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1925:4555 CAPLUS

DOCUMENT NUMBER: 19:4555 ORIGINAL REFERENCE NO.: 19:637g-i

TITLE: Hydantoins. XLIII. Synthesis of the

polypeptide-hydantoin: "hydantoin-3-acetic acid."

AUTHOR(S): Johnson, T. B.; Renfrew, Alice G.
SOURCE: Journal of the American Chemical Society (1925), 47,

240-5

CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB SCNCH2CO2Et (I) (for which a practical method of preparation is given) reacts with EtOH after heating 9 hrs. at 125° to give di-Et

thioncarbamoacetate, bi0 135-40° (with considerable decomposition). I and H2NCH2CO2Et in anhydrous Et20 give a mixture of di-Et thioureadiacetate (II), m. 85-7°, and the mono-Et ester, m. 96°, separated from II by its greater solubility in 50% AcCH. Either ester with HCl yields 2-thiohydantoin-3-acetic acid (III), yellow, m. 210-2° to a yellow oil; the alkali solution is wine-red. This is desulfurized by C1CH2CO2H, giving hydantoin-3-acetic acid, m. 190-1°. III is also obtained in

good yield from I and H2NCH2CO2H after repeated evaporation with HCl. 871893-67-3P, Hydantoin, 5-[bromo(2,3,4,5-tetrahydro-2,5-diketo-4-

methyl-4-imidazolyl)methylene]-RL: PREP (Preparation)

(preparation of) RN 871893-67-3 CAPLUS

RN 871893-67-3 CAPLUS CN Hydantoin, 5-[bromo(2,3,4,5-tetrahydro-2,5-diketo-4-methyl-4-

imidazolyl) methylene] - (2CI) (CA INDEX NAME)

=> D IBIB ABS HITSTR L30 1067

L30 ANSWER 1067 OF 1069 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1925:4556 CAPLUS

DOCUMENT NUMBER: 19:4556

ORIGINAL REFERENCE NO.: 19:637i

TITLE: Hydantoins. XLIV. Pyvuril and dipyruvic triureide AUTHOR(S): Davidson, David

SOURCE: Journal of the American Chemical Society (1925), 47,

255-9 CODEN: JACSAT: ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable
AB Pyvuril (Grimaux, Ann. chim. phys. [5] 11, 367) reacts with 1 mol. Br in

AcOH to give CO(NH2)2 and bromopyruvic ureide and with 2 mols. to give CO(NH2)2 and the di-Br derivative This is analogous to the action of HNO3. HI gives 5-methylhydantoin, which confirms the intermediate existence of pyruvic monoureide; this has not been isolated on account of its

reactivity, undergoing polymerization to dipyruvic acid. Concentrated H2SO4 given dipyruvic ureide, m. 290°, whose Br derivative, C8H7BrN404, m. 265° (decomposition). Similar results were obtained with dipyruvic

triureide.
1871893-67-3P, Hydantoin, 5-[bromo(2,3,4,5-tetrahydro-2,5-diketo-4-methyl-4-imidazolyl)methylene]-

RL: PREP (Preparation) (preparation of)

RN 871893-67-3 CAPLUS

CN Hydantoin, 5-[bromo(2,3,4,5-tetrahydro-2,5-diketo-4-methyl-4imidazolyl)methylenel- (2CI) (CA INDEX NAME)

=> D IBIB ABS HITSTR L30 1066

L30 ANSWER 1066 OF 1069 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1925:6026 CAPLUS

DOCUMENT NUMBER: 19:6026

ORIGINAL REFERENCE NO.: 19:830a-f

TITLE: The metabolism of tryptophan, I. The synthesis of

racemic bz-3-methyltryptophan

AUTHOR(S):

Journal of Biological Chemistry (1924), 62, 495-514 SOURCE:

Robson, Wm. CODEN: JBCHA3; ISSN: 0021-9258

DOCUMENT TYPE: Journal

LANGUAGE:

Unavailable A good yield of p-tolylhydrazine is to be obtained only if the temperature is kept at 0-2°. This was then combined with AcCO2H to yield pyruvic acid p-tolylhydrazone, m. 159° (yield 88%), which was treated in 7 parts absolute EtOH at 65-70° with a rapid stream of dry HCl. After 2 hrs. the mixture was allowed to cool and was then poured into a large volume of H2O. After filtering and drying, it was distilled 2-Carboxy-5methylindole, b4.0 236°, m. 163° (yield 60%). This was hydrolyzed with EtOH-KOH, the acid liberated by acidification and extracted with Et20. The Et20 solution was dried with Na2SO4, filtered and then treated with a rapid stream of dry NH3. NH4 5-methylindole-2-carboxylate began to sep. as a light vellow powder almost immediately. After saturation, the mixture was allowed to stand 2 or 3 hrs. and was then filtered. Ten g. of the dry NH4 salt were then placed in a 1-1. flask and heated, under a long air condenser, at 230-40° for 30 min. After distillation in steam, 5-methylindole, m. 58.5°, separated, yield 3.9 g. This could be converted into 5-methylindole-3-aldehyde, m. 148°, by Ellinger and Flamand's method (C. A. 1, 2480), with a yield of 1.2 g. from 9 g. methylindole, and a recovery of 4.6 g. unchanged methylindole and the formation of 3-chloro-6-methylquinoline, m. 85.5°, has an odor resembling lilac. A 1.15 g. yield of a purer 5-methylindole-3-aldehyde, m. 151°, was obtained by the method of Majima and Kotake (C. A. 17, 1017) from 6.5 g. methylindole but no unchanged methylindole was recovered. In a 3rd method, 2-carbethoxy-5-methylindole was converted into 2-carboxy-5-methylindole-3-aldehyde, m. 189°, by Adams and Levine's modification of the Gatterman method (C. A. 17, 3867). On hydrolysis with 40% NaOH for 15 min. and reacidification, 2-carboxy-5-methylindole-3-aldehyde was precipitated After solution in NH°40H and repptn. this turned brown at 235° and decomposed violently at 254-5°. Attempts at the preparation of 5-methylindole-3-aldehyde from this were unsuccessful. 5-Methylindolalhydantoin, from the 3-aldehyde, hydantoin, NaOAc and Ac20 (cf. Majima and Kotake, loc. cit.) m. 295-8°. This in 0.5 NaOH was reduced with Na-Hg to 5-methylindolylhydantylmethane, m. 206-7°. This was then hydrolyzed with Ba(OH)2, the Ba precipitated with H2SO4, and the bz-3-methyltryptophan, precipitated with HgSO4. The precipitate was filtered

out.

decomposed in dilute Ba(OH)2 with H2S, filtered, the Ba removed with H2SO4 and the filtrate evaporated in vacuo. EtOH precipitated a semicryst, mass, which

was

redissolved in H2O, repptd. with EtOH, and recrystd. from 50% EtOH. Yield 0.39 g. from 1.2 g. of the hydantylmethane. bz-3-Methyltryptophan, m. 259-63°, gives a beautiful purple with the Hopkins-Cole reagent; a purple color, which may be extracted with BuOH, with Br2-H2O; a strong reaction with triketohydrindene hydrate and is very bitter.

857767-36-3P, Hydantoin, 5-(5-methyl-3-indylmethylene)-

RL: PREP (Preparation) (preparation of)

RN 857767-36-3 CAPLUS

2,4-Imidazolidinedione, 5-[(5-methyl-1H-indol-3-yl)methylene]- (CA INDEX

NAME)

=> D IBIB ABS HITSTR L30 1065

L30 ANSWER 1065 OF 1069 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1925:7147 CAPLUS

DOCUMENT NUMBER: 19:7147 ORIGINAL REFERENCE NO.: 19:973b-d

TITLE:

Hydantoins, XLV, Dipyruvic ureide Davidson, David: Johnson, T. B. AUTHOR(S):

SOURCE: Journal of the American Chemical Society (1925), 47,

CODEN: JACSAT: ISSN: 0002-7863

DOCUMENT TYPE: Journal LANGUAGE: Unavailable

GI For diagram(s), see printed CA Issue. cf. C. A. 19, 637. Dipyruvic ureide (I), HN.CO.NH.CO.C:CHCMe.CO.NH.CO.NH,

may be obtained from pyruvil or dipyruvic triureide by the action of H2SO4, HBr or HCl; 6.4 g. result by adding to 10 g. pyruvic acid and 15 g. CO(NH2)2 in 15 cc. concentrated HCl, after 36 hrs., 17 g. concentrated H2SO4. Reduction with Pt and H in glacial AcOH gives the hydro derivative, C8H10O4N4, m. about 300° (decomposition). I (4.5 g.) in 25 cc. glacial AcOH, treated on the H2O bath with 2 cc. Br, gives about 5 g. Br derivative (II), C8H7O4N4Br, decomps. about 265-70°. Warming I with Br water gives

bromomethenyl-5'-[5'-methyl]hydantoin-5-hydantoic acid, crystallizing with

3H2O,

which is lost on the hot plate, giving feathery needles of the anhydrous compound Heated on the steam bath with concentrated H2SO4, II is formed. Br water reacts with II to give the di-Br derivative, hexagonal plates, m. about 250° (decomposition); soluble in about 17 parts boiling H2O. Concentrated HNO3 gives with I nitropyruvic ureide and parabanic acid.

861323-75-3P, Hydantoin, 5-[(2,3,4,5-tetrahydro-2,5-diketo-4methyl-4-imidazolyl)methylenel- 871893-67-3P, Hydantoin, 5-[bromo(2,3,4,5-tetrahydro-2,5-diketo-4-methyl-4-imidazolyl)methylene]-RL: PREP (Preparation)

(preparation of) 861323-75-3 CAPLUS RN

Hydantoin, 5-[(2,3,4,5-tetrahydro-2,5-diketo-4-methyl-4-CN imidazolvl) methylenel- (2CI) (CA INDEX NAME)

871893-67-3 CAPLUS

CN Hydantoin, 5-[bromo(2,3,4,5-tetrahydro-2,5-diketo-4-methyl-4imidazolvl) methylene] - (2CI) (CA INDEX NAME)

=> D IBIB ABS HITSTR L30 1064

L30 ANSWER 1064 OF 1069 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1928:4734 CAPLUS

22:4734 DOCUMENT NUMBER:

ORIGINAL REFERENCE NO.: 22:588f-i,589a

TITLE: Some pyrrole derivatives. II

AUTHOR(S): Kuster, Wm.; Koppenhofer, G. SOURCE:

Z. physiol. Chem. (1927), 172, 126-37

DOCUMENT TYPE: Journal

LANGUAGE:

Unavailable AB Synthetic pyrrylamino acids are of interest in connection with the study of the prosthetic group of the blood pigment. The condensation of formylpyrrole derivs. with diketopiperazine, followed by hydrogenation and opening of the anhydride ring, affords a method for preparing alanine derivs. of this type. 2,2-Di[3,5-dimethyl-4-carbethoxypyrral]-2,5diketopiperazine (I), red crystals, m. 268-9°, was obtained in 60% yield by refluxing a mixture of 3,5-dimethyl-4-carbethoxy-2-formylpyrrole and glycine anhydride with AcOH and NaOAc. Its di-Me derivative, red crystals, m. 156°, was prepared by treating the Ag salt of I with MeI. Reduction of I in EtOH by Al-Hg and neutralization with dilute H2SO4 gave an almost quant. yield of colorless 2,2-di[3,5-dimethyl-4carbethoxypyrrylmethyl]-2,5-diketopiperazine (II), m. 122°. Attempts to prepare a monopyrral derivative of diketopiperazine were unsuccessful, both CH2 groups of the latter being equally reactive. Hydrolysis of II by Ba(OH)2 gave 55% of $\beta-[3,5-dimethyl-4$ carbethoxypyrry1-2]-alanine (III), which decomps. 180-6° and does not form a Cu salt. Another method of preparing III consists in condensing the formylpyrrole with rhodanin, hydrolyzing the rhodanin ring, converting the resulting thicketonic acid into the oxime and reducing the latter. 3,6-Dimethyl-4-carbethoxy-2-pyrralrhodanin (IV), red needles, m. 253-5°, was obtained in 80% yield by refluxing the formylpyrrole and rhodanin with AcOH and NaOAc; phenylhydrazone, red needles, m.

272-5° (decomposition). Hydrolysis of IV by Ba(OH)2 converted it into 3,5-dimethyl-4-carbethoxy-2-pyrrylthiopyruvic acid (V), decomps. 196°; oxime, m. 218°. Reduction of the oxime by Na-Hg in the presence of lactic acid gave 62% of III. Hydrolysis of the CS group in V by heating in a sealed tube with C1CH2CO2H converted it into 3,5-dimethyl-4-carbethoxy-2-pyrrylpyruvic acid, m. 192°. 1-Phenv1-2,5-dimethv1-3-carbethoxypyrrole was condensed with aminoacetal by heating with concentrated HCl, forming di[1-phenyl-2,5-dimethyl-3-carbethoxy-4-pyrryl]-β-aminoethane, m. 246°. Similarly, 1-phenyl-2,5-dimethyl-4-carbethoxypyrrole with CH2O and HCl yielded di[1-phenyl-2,5-dimethyl-4-carbethoxy-3-pyrryl]methane, m. 102°. 856076-91-0P, 3-Pyrrolecarboxylic acid, 5-(2,3-dihydro-4-keto-2thicketo-5(4)-thiazylidenemethyl)-2,4-dimethyl-, ethyl ester RL: PREP (Preparation) (preparation of) 856076-91-0 CAPLUS INDEX NAME NOT YET ASSIGNED

RN

CN

=> D IBIB ABS HITSTR L30 1063

L30 ANSWER 1063 OF 1069 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1938:14713 CAPLUS DOCUMENT NUMBER: 32:14713

ORIGINAL REFERENCE NO.: 32:2114h-i,2115a-c

Synthesis of r-6-methoxytryptophan and of harmine, TITLE:

with a note on the action of acetaldehyde on tryptophan

AUTHOR(S): Harvey, Douglas G.; Robson, Wm.

SOURCE: Journal of the Chemical Society (1938) 97-101

CODEN: JCSOA9; ISSN: 0368-1769

DOCUMENT TYPE: Journal LANGUAGE:

Unavailable

OTHER SOURCE(S): CASREACT 32:14713

Details are given of the preparation of the following intermediates: o-nitro-p-cresol, o-nitro-p-tolyl Me ether, the K derivative of Et o-nitro-p-methoxyphenyl-pyruvate, NH4 6-methoxyindole-2-carboxylate, 6-methoxyindole and 6-methoxyindole-3-aldehyde (I) (the last being accompanied with some 3-chloro-7-methoxy-quinoline). Heating 3.5 g. I, 2.3 g. hydantoin and 10 ml. piperidine under reflux for 35 min. gives 3.7 g. 5-(6'-methoxyindolal)-hydantoin (II), yellow, m. 311-15°; it gives, when heated with Ehrlich's reagent, a very pale pink color which fades rapidly on cooling. Reduction of 1 g. of II in pyridine with H2S by heating at 100° for 70 hrs. gives 0.45 g. of 5-(6'-

methoxyindolylmethyl)hydantoin, m. 220° (50% yield on basis of recovered II); cleavage by heating with dilute NH4OH at 100-10° for 72 hrs. gives 60% of 6-methoxytryptophan (III), m. 263-8°, decomps. 274°; it has an intensely sweet taste, gives a greenish blue color with the Hopkins-Cole reagent, changed to purplish red with FeC13 and to a vivid green-blue on dilution; Br in H2O gives a characteristic rose-pink color, readily removed by AmOH or BuOH; attempted demethylation with HCl or H2SO4 gives dark brown or green amorphous products. It would appear that before the HO derivative (which, with III, is considered a biol. precursor of the Harmala alkaloids), can be obtained, a new method of synthesizing tryptophan (IV) will be necessary. 1-IV and AcH in H2O, 12 hrs. at room temperature, give a quant. yield of 3-methyl-3,4,5,6-tetrahydro-4carboline-5-carboxylic acid (V), m. 295-9°; oxidation gives 70% of harman. Similarly, III and AcH in H2O, gently warmed for 10 min., give the 11-MeO derivative of V, with 1 mol. H2O, m. 244-6°; oxidation gives 40% of harmine. Attempts to decarboxylate V have been unsuccessful, which would indicate that the tetrahydropyridine ring is formed after, rather than before decarboxylation has occurred. 858786-93-3P, Hydantoin, 5-(6-methoxy-3-indolylmethylene)-

IT 858786-93-3P, Hydantoin, 5-(6-methoxy-3-indolylmethylene)-RL: PREP (Preparation)

(preparation of) RN 858786-93-3 CAPLUS

CN 2,4-Imidazolidinedione, 5-[(6-methoxy-1H-indol-3-y1)methylene]- (CA INDEX NAME)

=> D IBIB ABS HITSTR L30 1062

L30 ANSWER 1062 OF 1069 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1939:8714 CAPLUS

DOCUMENT NUMBER: 33:8714

ORIGINAL REFERENCE NO.: 33:1316h-i,1317a

TITLE: Synthesis of $r-\alpha$ -methylamino- β -3-indolylpropionic acid

AUTHOR(S): Miller, Eric J.; Robson, Wm.

SOURCE: Journal of the Chemical Society (1938) 1910-12

CODEN: JCSOA9; ISSN: 0368-1769

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB Glycine (19 g.) in 375 ml. of 2 N NaOH and 40 mols. of PhSO2CI (mixed with shaking), treated with 25 g. of solid NaOH and 48 ml. Me2SO4, give 87.5% of N-benzenesulfonylsarcosine (1). I (40 g.), refluxed with 95 ml. 50% H2SO4 for 4-5 hrs., gives 1-methylglycine which with 14 g. KCNO yields 72% of 1-methylhydantoin (II), m. 157-9°. Refluxing 5 g. of indole-3-aldehyde, 5 g. II and 10 ml. piperidine for 1 hr. gives a quant. yield of 5-(3'-indolal)-1-methylhydantoin (III), m. 337-8°.

Reduction of III with H2S and concentrated NH4OH (heating at 100-5° for 3 days and repeating the procedure twice) gives 80% of the 5-(3'-indolylmethyl) derivative, m. 211-12°, which was hydrolyzed by refluxing with Ba(OH)2 for 20 hrs., giving 90% of α -methylamino- β -3-indolylpropionic acid, m. 245° (decomposition). 91902-09-9P, Hydantoin, 5-(3-indolylmethylene)-1-methyl-

IT 91902-09-9P, Hydantoin, 5-(3-indolylmethylene)-1-methyl-RL: PREP (Preparation) (preparation of)

RN 91902-09-9 CAPLUS

CN Hydantoin, 5-(indol-3-ylmethylene)-1-methyl- (7CI) (CA INDEX NAME)

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